

2-Isopropyl-6-methyl-4-pyrimidone
2814-20-2 | DTXSID1027502

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 273 °C

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

Image not found

N,N-Dimethyl-p-phenylenediamine

Measured: 263

Predicted: 267

Image not found

1,2-Benzenediamine, N,N-dimethyl-

Measured: 218

Predicted: 267

Image not found

1,3-Benzenediamine, N,N-dimethyl-

Measured: 270

Predicted: 267

Image not found

4-Nitroaniline

Measured: 332

Predicted: 282

Image not found

3-Nitroaniline

Measured: 306

Predicted: 285